



# Institute for Materials Science

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## Institute for Materials Science Lecture Series



**Professor Udo Schwingenschlögl**  
**King Abdullah University, Materials Science & Engineering**

### **Insights Into Two-Dimensional Materials from First-Principles Calculations**

**Wednesday, July 22, 2015**

**11 - 12**

**MSL Auditorium (TA-03 - Bldg 1698 - Room A103)**

**Abstract:** We discuss recent findings from first-principles calculations on the structural and electronic properties of two-dimensional materials. The focus of the talk is on silicene, the Si analogue of graphene, and on the class of monolayer transition metal dichalcogenides. For silicene, in particular the effects of the substrate and strategies for achieving a quasi-freestanding configuration are addressed. Moreover, we present quantitative insight into the interplay between the spin-orbit coupling and an external or internal magnetic field. For the transition metal dichalcogenides, we discuss how the valley polarization depends on the strength of the spin-orbit coupling and the exchange interaction. A huge valley drift is observed in MoS<sub>2</sub> under uniaxial strain, more than an order of magnitude larger than in graphene. We also demonstrate that breaking of the mirror symmetry results in a sizable Rashba splitting in the center of the Brillouin zone.

**Biography:** Udo Schwingenschlögl is a Professor in the Physical Sciences and Engineering Division of King Abdullah University of Science and Technology (KAUST).

Before joining KAUST in September 2008, he has worked at the International Center of Condensed Matter Physics in Brasilia, Brazil, and the University of Augsburg in Germany.

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For general information contact Caryll Blount, IMS Administrator  
caryll@lanl.gov \* 665-3950

*Hosted by Alexander Balatsky*  
*Director of the Institute for Materials Science (IMS)*